

**Supporting Information for “Transition State Energy Decomposition Study of Acetate-Assisted and Internal Electrophilic Substitution C-H Bond Activation by (acac-O,O)<sub>2</sub>Ir(X) Complexes (X = CH<sub>3</sub>COO, OH)”**

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**QChem 3.0.2.1 Full Reference (22)**

Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, R. A. DiStasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khaliullin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, Q-Chem, Version 3.1, Q-Chem, Inc., Pittsburgh, PA (2007).

Additional authors for Version 3.1:

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**B3LYP/LACVP\*\* Cartesian Coordinates**

**Benzene**

C1	-0.6983856129	1.2096393648	0.0000000000
C2	0.6983856129	1.2096393648	0.0000000000
C3	1.3967712258	0.0000000000	0.0000000000
C4	0.6983856129	-1.2096393648	0.0000000000
C5	-0.6983856129	-1.2096393648	0.0000000000
C6	-1.3967712258	0.0000000000	0.0000000000
H7	-1.2417993707	2.1508596029	0.0000000000
H8	1.2417993707	2.1508596029	0.0000000000
H9	2.4835987415	0.0000000000	0.0000000000
H10	1.2417993707	-2.1508596029	0.0000000000
H11	-1.2417993707	-2.1508596029	0.0000000000
H12	-2.4835987415	0.0000000000	0.0000000000

**Methane**

C1	-0.0481074598	-0.0000006806	-1.0242422733
H2	-1.0778071564	0.0000051314	-0.6602730061
H3	0.4665966393	0.8917667335	-0.6602261021
H4	0.4666024663	-0.8917665927	-0.6602248642
H5	-0.0482101455	0.0000028321	-2.1164157486

***cis*-(acac)<sub>2</sub>Ir(HOAc)(OAc)**

Ir1	0.1763789913	-0.0454950249	0.1156011060
O2	0.0464091196	-0.4642930857	2.0884554354
O3	2.2067962049	-0.2539526625	0.3101819412
O4	-0.1723999442	-2.0271299116	-0.2327923888
O5	-1.8323870156	0.2198973157	-0.1438986640
C6	-1.0914404164	-0.6000395500	2.6530606956
H7	-1.0195305090	-0.8685833716	3.7124319597
C8	-2.6469379587	-0.0380710274	0.8033451235
H9	-3.7000409464	0.0953892952	0.5302117819
C10	2.7499764934	-1.4041455828	0.2430604491
H11	3.8366026084	-1.3933158141	0.3902494754
C12	0.7852701053	-2.8698045503	-0.2129951384
H13	0.4681015662	-3.9029290800	-0.3970869741
C14	-2.3666196689	-0.4545481496	2.1066962997
H15	-3.2100140887	-0.6193299701	2.7673955535
C16	2.1477451909	-2.6452186216	0.0044330815
H17	2.7984906399	-3.5122442699	-0.0161150771
O18	0.3949331901	0.1860445409	-1.9708590242
C19	0.7280032008	1.2218884082	-2.5913881096
C20	0.8434675664	1.1780845015	-4.0891769596
H21	0.0989252132	1.8514670591	-4.5252118746
H22	1.8299042131	1.5419008917	-4.3898993535
H23	0.6841432881	0.1639868063	-4.4529525652
O24	0.9855627255	2.3672834048	-2.0430104572
O25	0.5503767767	1.9902115741	0.3573819300
H26	0.8513398108	2.3246970825	-1.0043482137
C27	-0.0399456220	2.7831520288	1.2594715297
C28	0.4312668163	4.2244489301	1.1496161680
H29	1.5092614627	4.2778675963	1.3316333204
H30	0.2483850991	4.6155905589	0.1433158289
H31	-0.0959335606	4.8364200082	1.8818193398
O32	-0.8417075749	2.4040956260	2.0881937690

**2**

SCF = -866.37821980454 (-866.61042869347)

Ir1	0.0379630000	-0.1000200000	-0.0225730000
O2	-0.0030570000	-0.1091010000	2.0166920000
O3	2.0748750000	-0.0648710000	0.1257860000

O4	-0.1221580000	-2.1239050000	0.1813390000
O5	-1.9933090000	-0.0677860000	-0.2438300000
C6	-1.1144330000	-0.1242240000	2.6451820000
H7	-1.0027130000	-0.1327190000	3.7354580000
C8	-2.7591080000	-0.0981120000	0.7736240000
H9	-3.8273050000	-0.0964920000	0.5272280000
C10	2.7320920000	-1.1376000000	0.3256080000
H11	3.8151080000	-0.9876500000	0.4056690000
C12	0.9162390000	-2.8431670000	0.3667130000
H13	0.6980000000	-3.9123790000	0.4682550000
C14	-2.4129310000	-0.1255080000	2.1298780000
H15	-3.2269350000	-0.1428210000	2.8457800000
C16	2.2538270000	-2.4478820000	0.4460560000
H17	2.9887940000	-3.2276020000	0.6113150000
O18	0.1909070000	0.3148910000	-2.0945330000
C19	0.2035870000	1.5731080000	-1.8631400000
C20	0.2676220000	2.5797070000	-2.9685370000
H21	-0.7518920000	2.8392590000	-3.2740850000
H22	0.7646460000	3.4864070000	-2.6194470000
H23	0.7895550000	2.1583530000	-3.8292450000
O24	0.1326450000	1.9239670000	-0.6344970000

#### 6M-TS-Benzene

Ir1	0.0426273741	-0.0291254467	-0.0780162842
O2	-0.1464724185	0.5552824178	2.9815866140
C3	1.0057692629	0.1626290554	2.6797738757
C4	2.0667616341	0.0720175259	3.7548203946
O5	1.3687187900	-0.1829225912	1.4969512245
H6	3.0013263906	-0.3186912881	3.3522536527
H7	2.2309033130	1.0665769714	4.1801700577
H8	1.7064258227	-0.5726857025	4.5614262454
C9	-0.6837929782	-2.7000038652	-0.9951958489
O10	-0.1031332927	-2.0737936170	-0.0492041814
H11	-0.6504357900	-3.7912296654	-0.8914481092
C12	1.1907451771	2.5835797815	-0.6957007595
O13	0.2477559216	2.0109840108	-0.0538689839
H14	1.1855874242	3.6763005022	-0.6066722299
C15	2.3800958625	0.6427333992	-1.7165282109
C16	2.1991753044	2.0106000557	-1.4739093621
H17	3.2252747922	0.3579204442	-2.3560440030
H18	2.9081551054	2.6892194641	-1.9348374613
O19	1.6928096513	-0.3410197297	-1.2960421183
C20	-1.4920069824	-0.8291376830	-2.4306561855
C21	-1.3466232080	-2.1836873670	-2.1136179193
H22	-2.0433527520	-0.5848655004	-3.3467724998
H23	-1.7835830222	-2.8996931348	-2.8007838450

O24	-1.0640262629	0.1904370732	-1.7975577577
C25	-4.0446369284	1.2767877288	0.6269258943
C26	-2.6535196247	1.3158073199	0.6184000995
C27	-1.8899878946	0.1818266191	0.9772382383
C28	-2.5852226050	-0.9829022204	1.3762841499
C29	-3.9756473343	-1.0259004744	1.3819504155
C30	-4.7064079480	0.1033803741	0.9999878348
H31	-4.6169198027	2.1556408083	0.3423857520
H32	-2.1340913237	2.2233104447	0.3291380752
H33	-0.9504367713	0.4106712629	1.7838018156
H34	-2.0147319366	-1.8495856267	1.6966029412
H35	-4.4934598132	-1.9307929495	1.6882834279
H36	-5.7930757899	0.0721469986	1.0046974060

#### 4M-TS-Benzene

Ir1	0.0069328269	-0.0047370597	0.0198713073
O2	0.0044441807	0.1414011823	3.8355964470
C3	0.8598895124	0.0691102555	2.9824787087
C4	2.1897969053	0.7919999314	3.0427371816
O5	0.7362655168	-0.7317409607	1.8907340269
H6	3.0087967677	0.0770381324	2.9230727738
H7	2.2619728126	1.5080347247	2.2185909026
H8	2.2819845204	1.3172499994	3.9944260989
C9	0.9215712000	-1.7972428169	-2.0793225629
O10	1.0062355011	-1.5765255439	-0.8268222664
H11	1.5456095937	-2.6282880463	-2.4282317723
C12	-0.4975483330	2.7808772887	0.7843911962
O13	-0.9398318756	1.5893621816	0.9069075170
H14	-1.1216838221	3.5347816668	1.2778746930
C15	1.5877567528	2.4341027479	-0.5438533383
C16	0.6517309945	3.2317989649	0.1300930645
H17	2.4448659477	2.9496988922	-0.9971130294
H18	0.8385220326	4.2997421866	0.1501271120
O19	1.5910343330	1.1725783769	-0.6975496466
C20	-0.7112495167	-0.0548965459	-2.7882512062
C21	0.1389610032	-1.1362899722	-3.0328987501
H22	-1.2732361255	0.3505563837	-3.6371451387
H23	0.1985209156	-1.4948955854	-4.0543902051
O24	-0.9376704342	0.5534701607	-1.6887610445
C25	-3.9535392643	-1.4856226924	1.2133260516
C26	-2.7765066897	-0.7437774115	1.1973661780
C27	-1.5544338682	-1.3264780805	0.7878580089
C28	-1.5628056417	-2.6926318417	0.4181474555
C29	-2.7376505278	-3.4379701349	0.4390592492
C30	-3.9345073596	-2.8297655130	0.8283828261
H31	-4.8861450434	-1.0238968516	1.5256656466

H32	-2.7834704322	0.2974387491	1.5007914738
H33	-0.5376031467	-1.1278484922	1.6054800968
H34	-0.6265439512	-3.1636107663	0.1351884645
H35	-2.7265221543	-4.4874205898	0.1575650107
H36	-4.8546855284	-3.4086817031	0.8421785201

#### 6M-TS-Methane

Ir1	0.0313481016	-1.3363562995	-0.1693895078
C2	0.1002964199	-3.5062862634	-0.8506825438
H3	-0.2343156756	-3.2515742139	0.4522013014
O4	-0.6080268584	-3.5875375150	1.7375618134
C5	-0.8154679008	-2.5001808198	2.3365677375
C6	-1.2761788031	-2.5121795861	3.7729152387
O7	-0.6529960860	-1.3578077328	1.7833531187
H8	-1.4353092872	-1.4989141853	4.1413260485
H9	-2.2013131343	-3.0904199730	3.8500919106
H10	-0.5229082981	-3.0167058861	4.3851048570
C11	2.9461190087	-1.2664853704	-0.1889562824
O12	1.9390626627	-1.4337535342	0.5708539195
H13	3.9100712661	-1.3163010652	0.3313361345
C14	-2.5316998940	-0.1772295968	-0.9410008650
O15	-1.9000023706	-1.2808718631	-0.8479274928
H16	-3.5557845576	-0.2840560521	-1.3179316896
C17	-0.8255358644	1.4610360623	-0.1573987249
C18	-2.0942023366	1.1147843729	-0.6344718035
H19	-0.6329639173	2.5250812759	0.0274830267
H20	-2.8005286782	1.9230366801	-0.7872746308
O21	0.1659323331	0.7041596421	0.0986298714
C22	1.8612220839	-0.9311435794	-2.4097047716
C23	2.9742481713	-1.0337763416	-1.5704102290
H24	2.0497142002	-0.7349721094	-3.4720439306
H25	3.9493046764	-0.9122147944	-2.0287812567
O26	0.6248221795	-1.0402690718	-2.1160406751
H27	-0.5670922399	-3.3717073030	-1.7003646053
H28	-0.1449830215	-4.4895391077	-0.4262668935
H29	1.1432701656	-3.5623183738	-1.1625914440

#### 4M-TS-Methane

Ir1	0.0043505673	0.0024705030	-0.0023968788
C2	0.0427901701	0.0011953805	2.2451205772
H3	1.1668535062	0.0020769293	1.4883300408
O4	2.9154200598	1.8394523330	1.4052048945
C5	2.8304968128	1.0973665146	0.4521847486
C6	3.5760796775	1.2840021244	-0.8509976024
O7	2.0786310089	-0.0376519997	0.4794366546
H8	4.1565686694	0.3854271504	-1.0796948378

H9	2.8620826582	1.4247120380	-1.6687145847
H10	4.2338219612	2.1512161623	-0.7824662493
C11	-0.8758901157	-2.7579647516	-0.2216374914
O12	0.1579952014	-2.0342554015	-0.0582632834
H13	-0.6647641771	-3.8324372133	-0.2711016298
C14	-0.2254629708	2.7444346277	-0.9811006837
O15	-0.1088594337	2.0478163133	0.0808886871
H16	-0.3128567710	3.8210035903	-0.7951713593
C17	-0.1475246355	0.9966328619	-2.7620005341
C18	-0.2441328054	2.3199569520	-2.3141100964
H19	-0.1727680341	0.8330984432	-3.8466768396
H20	-0.3469690031	3.0887154153	-3.0717918018
O21	-0.0240913559	-0.0700415265	-2.0772226757
C22	-2.6834024693	-1.0445962827	-0.2954230312
C23	-2.2147747282	-2.3584455724	-0.3340581401
H24	-3.7637570972	-0.8880669206	-0.3885318873
H25	-2.9534524693	-3.1414354372	-0.4629163287
O26	-2.0214665335	0.0407737429	-0.1587051565
H27	-0.6304656377	0.8428195506	2.3994685679
H28	0.8861476017	0.1911286346	2.9326171611
H29	-0.3943643376	-0.9546164354	2.5310839896

## 2TS-Benzene

Ir	-0.099357	0.015321	0.007757
O	0.035599	-0.144141	2.888354
C	1.207883	-0.168182	2.495877
C	2.377219	-0.221375	3.458723
O	1.530747	-0.129845	1.235452
H	3.303397	-0.490068	2.948397
H	2.498895	0.762502	3.924341
H	2.159739	-0.937721	4.254263
C	-0.551953	-2.540121	-1.318390
O	0.062706	-1.994004	-0.343162
H	-0.322117	-3.604937	-1.443689
C	0.433843	2.856062	-0.208230
O	-0.243530	2.002300	0.442723
H	0.281335	3.894046	0.108564
C	1.638955	1.381476	-1.805517
C	1.330136	2.623392	-1.264469
H	2.352552	1.340329	-2.633886
H	1.821218	3.486217	-1.699207
O	1.202566	0.217332	-1.480385
C	-1.929066	-0.653193	-2.181135
C	-1.463321	-1.972227	-2.213220
H	-2.684239	-0.369025	-2.924085
H	-1.872864	-2.621873	-2.978768

O	-1.599363	0.287331	-1.388439
C	-4.628612	-0.400283	0.157932
C	-3.832913	0.509715	0.848040
C	-2.737832	0.057635	1.597645
C	-2.444553	-1.312952	1.647256
C	-3.248108	-2.224224	0.948995
C	-4.336413	-1.769857	0.209417
H	-5.480145	-0.050559	-0.420265
H	-4.058100	1.571595	0.806977
H	-2.133234	0.749209	2.173731
H	-1.612431	-1.649781	2.254008
H	-3.024459	-3.286715	0.993059
H	-4.962337	-2.476947	-0.328737

### 2TS-Methane

Ir	-0.070877	-0.067497	0.031324	56.303487
C	0.557638	-0.131887	3.290417	-6.090284
H	1.031237	0.059858	2.312725	-2.074006
O	2.629716	1.103954	1.203145	-3.170477
C	2.607431	1.144226	-0.021937	0.552640
C	3.691212	1.823034	-0.847079	-4.473906
O	1.666627	0.624921	-0.773994	-3.070049
H	3.243323	2.573429	-1.505364	0.101853
H	4.423673	2.291650	-0.188860	-2.231747
H	4.187988	1.086617	-1.486487	0.094969
C	-0.260944	-2.968367	-0.247578	-0.263028
O	0.566162	-1.999278	-0.183842	-0.457009
H	0.206392	-3.934514	-0.469825	-2.550026
C	-0.855705	2.617423	-0.687307	-2.655152
O	-0.591591	1.877950	0.309499	-2.624260
H	-1.050991	3.665875	-0.437271	-0.151038
C	-0.812800	0.942254	-2.517430	0.299244
C	-0.940905	2.237811	-2.038485	-4.942478
H	-0.953848	0.765590	-3.587357	-2.322840
H	-1.164937	3.012896	-2.761954	0.049576
O	-0.567850	-0.149409	-1.879554	-0.602903
C	-2.394788	-1.839352	0.343944	0.216283
C	-1.647783	-2.949565	-0.060942	-4.203607
H	-3.465911	-1.990021	0.524489	0.102001
H	-2.177800	-3.887006	-0.185534	-2.502053
O	-1.990603	-0.648127	0.561381	-2.757558
H	-0.460424	-0.519983	3.207982	0.086594
H	0.545269	0.819514	3.825817	0.101568
H	1.186193	-0.854859	3.815624	0.059267

### 3-Benzene

C	-0.062783	0.047021	0.093723
C	-0.025768	0.009623	1.471194
C	1.224286	0.004476	2.146977
C	2.423246	0.051763	1.403971
C	2.356098	0.088932	-0.016453
C	1.136750	0.084243	-0.656126
Ir	2.275877	-2.247139	2.248542
O	3.912672	-2.464690	1.033376
C	5.049572	-1.815062	1.132959
O	5.289694	-0.853926	1.858168
O	0.637842	-2.412293	3.532067
C	-0.402938	-3.045655	3.154860
C	-0.692661	-3.595202	1.902917
C	0.130846	-3.553811	0.769223
O	1.288741	-3.046037	0.635713
O	3.243502	-1.440472	3.859780
C	3.846022	-2.178255	4.697840
C	3.955059	-3.577354	4.702105
C	3.373322	-4.441820	3.778234
O	2.656651	-4.172042	2.751003
C	6.110032	-2.406149	0.207865
H	5.693623	-2.599390	-0.784189
H	6.960378	-1.726191	0.139718
H	6.448814	-3.366680	0.610501
H	-1.166288	-3.155883	3.935674
H	-0.259611	-4.013992	-0.146841
H	4.330314	-1.629283	5.512995
H	3.524516	-5.516915	3.923958
H	-1.648491	-4.096162	1.795353
H	4.525142	-4.026878	5.507007
H	-0.944767	0.000947	2.048836
H	1.253633	0.131615	3.223107
H	3.379918	0.204469	1.892987
H	3.279982	0.138555	-0.582871
H	1.088918	0.120401	-1.740789
H	-1.018366	0.057658	-0.423844

### 3-Methane

Ir	-0.013561	-1.306328	-0.059409
C	-0.013113	-3.665396	-0.959784
H	-0.107062	-3.198241	0.088656
O	-0.506348	-3.611093	2.048398
C	-0.826044	-2.510715	2.493779
C	-1.324875	-2.330295	3.918777
O	-0.771658	-1.377445	1.834792
H	-2.224206	-1.709116	3.935867



H	-1.528308	-3.304418	4.364868
H	-0.558976	-1.814962	4.507644
C	2.906076	-1.286341	-0.006060
O	1.874638	-1.459169	0.719739
H	3.851939	-1.372865	0.541560
C	-2.561326	-0.128669	-0.808664
O	-1.921850	-1.227859	-0.781298
H	-3.581205	-0.211557	-1.200641
C	-0.852037	1.438512	0.083543
C	-2.117899	1.140658	-0.414557
H	-0.633517	2.480226	0.338696
H	-2.815938	1.963788	-0.513682
O	0.141354	0.657155	0.293517
C	1.898814	-0.863624	-2.249230
C	2.982258	-1.010808	-1.377807
H	2.126638	-0.641016	-3.298957
H	3.973790	-0.892363	-1.800183
O	0.652871	-0.963177	-1.996295
H	-0.781518	-3.381953	-1.673723
H	-0.205043	-4.677766	-0.590771
H	0.985886	-3.610497	-1.385120

## 6

Ir	0.140765	0.028463	0.062700
O	0.009949	-1.047381	1.620775
C	0.795056	-1.835573	-2.072503
O	1.052123	-1.553411	-0.860412
H	1.346435	-2.701407	-2.457636
C	-0.454541	2.752394	0.890561
O	-0.766502	1.533412	1.106220
H	-1.009968	3.470441	1.504658
C	1.324621	2.527711	-0.847818
C	0.493842	3.267359	0.000568
H	2.045045	3.084758	-1.458002
H	0.611845	4.344932	-0.019459
O	1.382354	1.264158	-1.017595
C	-0.899031	-0.101069	-2.651013
C	-0.096571	-1.199726	-2.950705
H	-1.569769	0.268458	-3.434702
H	-0.180331	-1.611351	-3.950179
O	-0.985888	0.563168	-1.559522
H	-0.419197	-0.543130	2.333688

## 6-Benzene

Ir	-0.151337	-0.198654	0.122846
O	1.079438	-0.458221	1.690878

C	0.548307	-2.000256	-2.070406
O	0.804377	-1.744709	-0.844159
H	1.185160	-2.785371	-2.496515
C	-0.493047	2.599937	0.921268
O	-0.958940	1.430628	1.093464
H	-1.004768	3.375275	1.504186
C	1.322372	2.167257	-0.708087
C	0.561904	3.010120	0.096708
H	2.124495	2.614071	-1.305452
H	0.809614	4.065271	0.089253
O	1.222149	0.901826	-0.867008
C	-1.331628	-0.429402	-2.581867
C	-0.411605	-1.439051	-2.913759
H	-2.029713	-0.120921	-3.372525
H	-0.451376	-1.822203	-3.927835
O	-1.472856	0.181373	-1.480222
C	-3.855405	-1.329974	0.494178
C	-3.088691	-0.672438	1.431765
C	-1.769506	-1.118272	1.714755
C	-1.256940	-2.239679	1.031634
C	-2.065085	-2.911138	0.077758
C	-3.341522	-2.458954	-0.184365
H	-4.863325	-0.987608	0.277197
H	-3.480209	0.188240	1.963241
H	-1.214784	-0.707743	2.549947
H	-0.307986	-2.657597	1.344406
H	-1.674427	-3.787693	-0.429428
H	-3.962066	-2.974537	-0.912391
H	1.874945	-0.876618	1.333160

## 6-Methane

Ir	0.334342	0.118021	0.158982
O	1.306154	-0.348289	1.850200
C	1.177667	-1.744743	-1.928243
O	1.315158	-1.463496	-0.692718
H	1.796274	-2.588148	-2.258040
C	-0.248652	2.835147	1.006015
O	-0.666222	1.633860	1.091671
H	-0.874355	3.570008	1.524528
C	1.802652	2.515554	-0.359496
C	0.894601	3.302979	0.346237
H	2.662038	3.007955	-0.824234
H	1.094425	4.367462	0.389842
O	1.790408	1.249976	-0.563160
C	-0.523091	-0.075380	-2.676310
C	0.357339	-1.143163	-2.890105

H	-1.111772	0.263530	-3.539225
H	0.401813	-1.550819	-3.894064
O	-0.747333	0.563413	-1.598054
C	-1.687428	-1.479265	0.896329
H	-0.690620	-1.190376	1.314047
H	1.106234	0.344996	2.495861
H	-2.045244	-0.906388	0.040908
H	-1.604806	-2.533783	0.631604
H	-2.371172	-1.322908	1.733306

#### ES-TS-Benzene

Ir	0.009317	-0.000081	0.023684
O	0.790087	-0.629285	1.853459
C	0.859991	-1.811856	-2.095034
O	0.977135	-1.579761	-0.846232
H	1.467610	-2.654169	-2.447161
C	-0.443631	2.773022	0.855052
O	-0.903360	1.583821	0.965235
H	-1.045610	3.528953	1.373094
C	1.608796	2.410718	-0.515679
C	0.699078	3.214643	0.189286
H	2.471695	2.915127	-0.969450
H	0.909352	4.277682	0.227906
O	1.578357	1.155651	-0.702200
C	-0.767109	-0.059132	-2.798496
C	0.067750	-1.156045	-3.042368
H	-1.335594	0.338101	-3.648641
H	0.106584	-1.529560	-4.059744
O	-0.965355	0.560663	-1.704436
C	-3.963493	-1.506374	1.128564
C	-2.787780	-0.762428	1.174744
C	-1.544105	-1.351044	0.854655
C	-1.524124	-2.720809	0.507319
C	-2.697201	-3.468939	0.467630
C	-3.917186	-2.857463	0.771474
H	-4.915992	-1.040461	1.366361
H	-2.815893	0.287677	1.446327
H	-0.529792	-1.076142	1.586373
H	-0.569532	-3.188034	0.285833
H	-2.667824	-4.522102	0.201984
H	-4.835789	-3.438079	0.735802
H	0.704230	0.119493	2.463311

#### ES-TS-Methane

Ir	0.202737	0.077506	0.088257
O	0.928262	-0.593526	1.921700

C	1.089657	-1.749865	-1.999718
O	1.181366	-1.507348	-0.753214
H	1.691981	-2.604173	-2.330827
C	-0.318452	2.822944	0.927570
O	-0.765033	1.628300	1.014245
H	-0.945284	3.567585	1.431886
C	1.776619	2.492660	-0.384038
C	0.840824	3.281587	0.298717
H	2.648945	3.003674	-0.809085
H	1.040029	4.346115	0.350558
O	1.764624	1.236031	-0.583007
C	-0.502476	0.015044	-2.752049
C	0.329142	-1.086590	-2.971298
H	-1.044514	0.415929	-3.617098
H	0.389971	-1.464345	-3.985885
O	-0.734144	0.636054	-1.661421
C	-1.436218	-1.310714	0.921730
H	-0.303588	-1.032656	1.550810
H	0.770770	0.119226	2.560043
H	-1.953153	-1.048813	-0.005321
H	-1.301683	-2.395838	0.921618
H	-2.089871	-0.979437	1.734561